Atraton

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 7.68e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.50e-01

Confidence level: 4.96e-01

Nearest Neighbors from the Training Set

Image not found
Morphazinamide
Measured: 1.50
Predicted: 4.01e-01